



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2014 – 08:00 PM EDT

PDB ID : 4CFS  
Title : CRYSTAL STRUCTURE OF THE COFACTOR-DEVOID 1-H-3-HYDROXY-4- OXOQUINALDINE 2,4-DIOXYGENASE (HOD) CATALYTICALLY INACTIVE H251A VARIANT COMPLEXED WITH ITS NATURAL SUBSTRATE 1-H-3-HYDROXY-4- OXOQUINALDINE  
Authors : Bui, S.; Steiner, R.A.  
Deposited on : 2013-11-19  
Resolution : 1.94 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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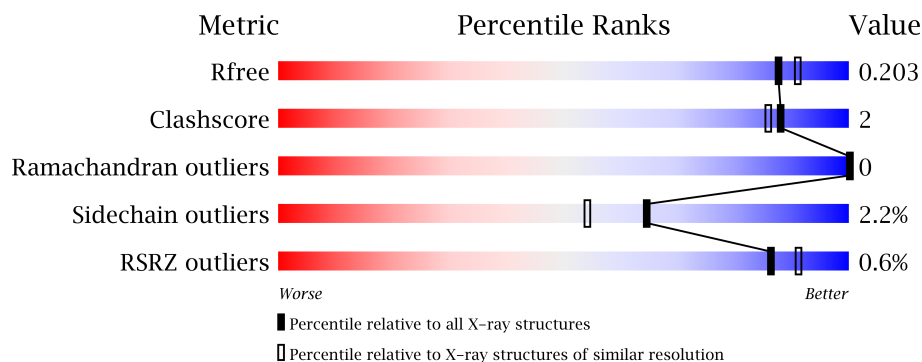
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 1.94 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2024 (1.96-1.92)
Clashscore	79885	2281 (1.96-1.92)
Ramachandran outliers	78287	2255 (1.96-1.92)
Sidechain outliers	78261	2255 (1.96-1.92)
RSRZ outliers	66119	2024 (1.96-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	287	
1	B	287	
1	C	287	
1	D	287	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	TAR	C	1279[A]	-	X
4	TAR	C	1279[B]	-	X
4	TAR	D	1279	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9772 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 1-H-3-HYDROXY-4-OXOQUINALDINE2,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	4	0
			2240	1434	389	409	8			
1	B	273	Total	C	N	O	S	0	6	0
			2262	1447	395	412	8			
1	C	273	Total	C	N	O	S	0	4	0
			2244	1434	389	412	9			
1	D	272	Total	C	N	O	S	0	6	0
			2252	1442	393	409	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP O31266
A	-9	ARG	-	EXPRESSION TAG	UNP O31266
A	-8	GLY	-	EXPRESSION TAG	UNP O31266
A	-7	SER	-	EXPRESSION TAG	UNP O31266
A	-6	HIS	-	EXPRESSION TAG	UNP O31266
A	-5	HIS	-	EXPRESSION TAG	UNP O31266
A	-4	HIS	-	EXPRESSION TAG	UNP O31266
A	-3	HIS	-	EXPRESSION TAG	UNP O31266
A	-2	HIS	-	EXPRESSION TAG	UNP O31266
A	-1	HIS	-	EXPRESSION TAG	UNP O31266
A	0	GLY	-	EXPRESSION TAG	UNP O31266
A	1	SER	-	EXPRESSION TAG	UNP O31266
A	2	MET	-	EXPRESSION TAG	UNP O31266
A	276	ASN	-	EXPRESSION TAG	UNP O31266
A	69	SER	CYS	ENGINEERED MUTATION	UNP O31266
A	251	ALA	HIS	ENGINEERED MUTATION	UNP O31266
B	-10	MET	-	EXPRESSION TAG	UNP O31266
B	-9	ARG	-	EXPRESSION TAG	UNP O31266
B	-8	GLY	-	EXPRESSION TAG	UNP O31266
B	-7	SER	-	EXPRESSION TAG	UNP O31266
B	-6	HIS	-	EXPRESSION TAG	UNP O31266

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	EXPRESSION TAG	UNP O31266
B	-4	HIS	-	EXPRESSION TAG	UNP O31266
B	-3	HIS	-	EXPRESSION TAG	UNP O31266
B	-2	HIS	-	EXPRESSION TAG	UNP O31266
B	-1	HIS	-	EXPRESSION TAG	UNP O31266
B	0	GLY	-	EXPRESSION TAG	UNP O31266
B	1	SER	-	EXPRESSION TAG	UNP O31266
B	2	MET	-	EXPRESSION TAG	UNP O31266
B	276	ASN	-	EXPRESSION TAG	UNP O31266
B	69	SER	CYS	ENGINEERED MUTATION	UNP O31266
B	251	ALA	HIS	ENGINEERED MUTATION	UNP O31266
C	-10	MET	-	EXPRESSION TAG	UNP O31266
C	-9	ARG	-	EXPRESSION TAG	UNP O31266
C	-8	GLY	-	EXPRESSION TAG	UNP O31266
C	-7	SER	-	EXPRESSION TAG	UNP O31266
C	-6	HIS	-	EXPRESSION TAG	UNP O31266
C	-5	HIS	-	EXPRESSION TAG	UNP O31266
C	-4	HIS	-	EXPRESSION TAG	UNP O31266
C	-3	HIS	-	EXPRESSION TAG	UNP O31266
C	-2	HIS	-	EXPRESSION TAG	UNP O31266
C	-1	HIS	-	EXPRESSION TAG	UNP O31266
C	0	GLY	-	EXPRESSION TAG	UNP O31266
C	1	SER	-	EXPRESSION TAG	UNP O31266
C	2	MET	-	EXPRESSION TAG	UNP O31266
C	276	ASN	-	EXPRESSION TAG	UNP O31266
C	69	SER	CYS	ENGINEERED MUTATION	UNP O31266
C	251	ALA	HIS	ENGINEERED MUTATION	UNP O31266
D	-10	MET	-	EXPRESSION TAG	UNP O31266
D	-9	ARG	-	EXPRESSION TAG	UNP O31266
D	-8	GLY	-	EXPRESSION TAG	UNP O31266
D	-7	SER	-	EXPRESSION TAG	UNP O31266
D	-6	HIS	-	EXPRESSION TAG	UNP O31266
D	-5	HIS	-	EXPRESSION TAG	UNP O31266
D	-4	HIS	-	EXPRESSION TAG	UNP O31266
D	-3	HIS	-	EXPRESSION TAG	UNP O31266
D	-2	HIS	-	EXPRESSION TAG	UNP O31266
D	-1	HIS	-	EXPRESSION TAG	UNP O31266
D	0	GLY	-	EXPRESSION TAG	UNP O31266
D	1	SER	-	EXPRESSION TAG	UNP O31266
D	2	MET	-	EXPRESSION TAG	UNP O31266
D	276	ASN	-	EXPRESSION TAG	UNP O31266
D	69	SER	CYS	ENGINEERED MUTATION	UNP O31266

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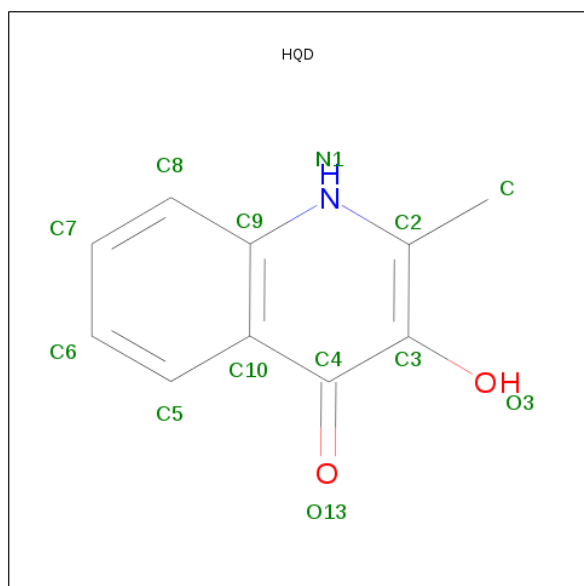
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Chain	Residue	Modelled	Actual	Comment	Reference
D	251	ALA	HIS	ENGINEERED MUTATION	UNP O31266

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

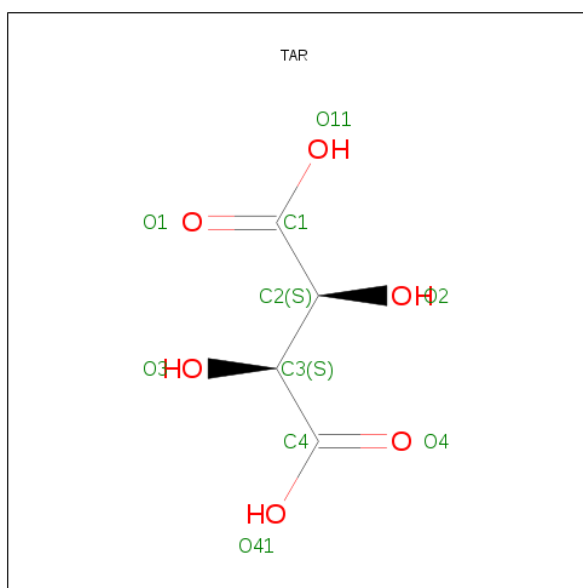
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0

- Molecule 3 is 3-HYDROXY-2-METHYLQUINOLIN-4(1H)-ONE (three-letter code: HQD) (formula: C<sub>10</sub>H<sub>9</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 13 10 1 2	0	0
3	B	1	Total C N O 13 10 1 2	0	0
3	C	1	Total C N O 13 10 1 2	0	0
3	D	1	Total C N O 13 10 1 2	0	0

- Molecule 4 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula:  $C_4H_6O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		
4	C	1	Total	C	O	0	0
			10	4	6		
4	C	1	Total	C	O	0	1
			20	8	12		
4	C	1	Total	C	O	0	0
			10	4	6		
4	D	1	Total	C	O	0	0
			10	4	6		
4	D	1	Total	C	O	0	0
			10	4	6		
4	D	1	Total	C	O	0	0
			10	4	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	159	Total	O	0	0
			159	159		
5	B	176	Total	O	0	0
			176	176		
5	C	125	Total	O	0	0
			125	125		
5	D	178	Total	O	0	0
			178	178		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 1-H-3-HYDROXY-4-OXOQUINALDINE2,4-DIOXYGENASE

Chain A: 



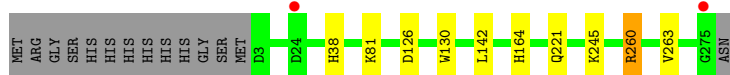
- Molecule 1: 1-H-3-HYDROXY-4-OXOQUINALDINE2,4-DIOXYGENASE

Chain B: 



- Molecule 1: 1-H-3-HYDROXY-4-OXOQUINALDINE2,4-DIOXYGENASE

Chain C: 



- Molecule 1: 1-H-3-HYDROXY-4-OXOQUINALDINE2,4-DIOXYGENASE

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.73Å 166.85Å 167.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.45 – 1.94 46.45 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.45-1.94) 98.5 (46.45-1.95)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.163 , 0.198 0.168 , 0.203	Depositor DCC
$R_{free}$ test set	4709 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 28.0	EDS
Estimated twinning fraction	0.511 for H, K, L 0.489 for -H, L, K 0.449 for -h,l,k	Xtriage
Reported twinning fraction	0.511 for H, K, L 0.489 for -H, L, K	Depositor
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	3 of 92719 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.5321e-03.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, HQD, TAR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.42	0/2322	0.62	2/3161 (0.1%)
1	B	0.46	0/2347	0.63	2/3192 (0.1%)
1	C	0.44	0/2326	0.62	2/3165 (0.1%)
1	D	0.44	0/2337	0.63	2/3180 (0.1%)
All	All	0.44	0/9332	0.62	8/12698 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	B	260	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	B	260	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	C	260	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	260	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	D	260	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	260	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	D	260	ARG	NE-CZ-NH1	5.93	123.27	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2240	0	2149	15	1
1	B	2262	0	2174	12	0
1	C	2244	0	2143	6	0
1	D	2252	0	2167	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	13	0	8	0	0
3	B	13	0	8	0	0
3	C	13	0	8	0	0
3	D	13	0	8	0	0
4	A	10	0	4	0	0
4	C	40	0	16	5	0
4	D	30	0	12	3	0
5	A	159	0	0	7	0
5	B	176	0	0	5	1
5	C	125	0	0	3	1
5	D	178	0	0	6	0
All	All	9772	0	8697	42	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (42) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:221[A]:GLN:OE1	5:A:2100:HOH:O	1.67	1.09
1:B:228:GLU:HG3	1:B:245[B]:LYS:HD3	1.45	0.98
1:B:273:ARG:NH1	5:B:2173:HOH:O	2.01	0.89
5:A:2108:HOH:O	4:C:1280:TAR:H3	1.71	0.89
4:D:1279:TAR:H3	5:D:2121:HOH:O	1.81	0.79
1:B:4:THR:HA	5:B:2001:HOH:O	1.80	0.79
1:A:260:ARG:HD3	1:D:165:ASP:OD2	1.84	0.78
1:A:165:ASP:OD2	1:C:260:ARG:HD3	1.91	0.69
1:A:8:GLU:OE1	5:A:2006:HOH:O	2.11	0.67
4:C:1279[B]:TAR:C4	4:C:1279[B]:TAR:O1	2.43	0.67
1:D:94:THR:HG22	5:D:2069:HOH:O	1.96	0.65
4:D:1278:TAR:H2	5:D:2126:HOH:O	1.96	0.65
1:B:245[A]:LYS:HG2	5:B:2146:HOH:O	1.98	0.64
1:D:4:THR:OG1	1:D:5:TYR:N	2.31	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:260:ARG:CD	1:D:165:ASP:OD2	2.52	0.57
1:B:138:LYS:NZ	5:B:2085:HOH:O	2.36	0.57
1:A:190:ARG:CD	1:B:77:GLN:HB3	2.35	0.56
1:D:164:HIS:HD2	4:D:1279:TAR:O41	1.88	0.56
1:C:164:HIS:HE1	5:C:2084:HOH:O	1.88	0.56
1:B:198:ARG:NH1	1:B:198:ARG:HB2	2.21	0.55
4:C:1279[A]:TAR:O2	4:C:1279[A]:TAR:O4	2.23	0.55
1:C:245:LYS:HE3	5:C:2107:HOH:O	2.06	0.54
1:B:150:ARG:NH1	5:B:2094:HOH:O	2.27	0.52
4:C:1279[B]:TAR:O4	4:C:1279[B]:TAR:C1	2.58	0.51
1:A:165:ASP:OD2	1:C:260:ARG:CD	2.59	0.50
4:C:1279[B]:TAR:O4	4:C:1279[B]:TAR:O1	2.30	0.47
1:B:198:ARG:CZ	1:B:198:ARG:HB2	2.44	0.47
1:A:266:ARG:HD3	5:A:2035:HOH:O	2.14	0.47
1:C:81:LYS:HG2	5:C:2042:HOH:O	2.15	0.46
1:D:27:GLY:HA3	5:D:2018:HOH:O	2.15	0.46
1:A:4:THR:HG23	1:A:5:TYR:CD1	2.51	0.46
1:A:198:ARG:NH1	5:A:2131:HOH:O	2.50	0.45
1:A:3:ASP:HA	5:A:2001:HOH:O	2.18	0.43
1:A:190:ARG:HD3	1:B:77:GLN:HB3	2.00	0.43
1:A:260:ARG:O	1:A:263[B]:VAL:HG22	2.19	0.43
1:A:164:HIS:HE1	5:A:2105:HOH:O	2.00	0.43
1:B:260:ARG:O	1:B:263:VAL:HG22	2.19	0.43
1:C:260:ARG:O	1:C:263:VAL:HG22	2.20	0.41
1:A:190:ARG:CZ	1:B:77:GLN:HG2	2.51	0.41
1:D:259:ASP:O	1:D:263[B]:VAL:HG23	2.20	0.41
1:D:199:ASN:ND2	5:D:2142:HOH:O	2.53	0.41
1:D:23:ARG:HD3	5:D:2014:HOH:O	2.21	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:2171:HOH:O	5:C:2076:HOH:O[3.644]	1.83	0.37
1:A:4:THR:OG1	1:A:208:ASN:OD1[1.655]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	275/287 (96%)	268 (98%)	7 (2%)	0	100	100
1	B	277/287 (96%)	270 (98%)	7 (2%)	0	100	100
1	C	275/287 (96%)	267 (97%)	8 (3%)	0	100	100
1	D	276/287 (96%)	267 (97%)	9 (3%)	0	100	100
All	All	1103/1148 (96%)	1072 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/246 (97%)	231 (97%)	7 (3%)	55	40
1	B	240/246 (98%)	234 (98%)	6 (2%)	60	48
1	C	238/246 (97%)	232 (98%)	6 (2%)	60	48
1	D	239/246 (97%)	233 (98%)	6 (2%)	60	48
All	All	955/984 (97%)	930 (97%)	25 (3%)	64	45

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	126	ASP
1	A	130	TRP
1	A	142	LEU
1	A	198	ARG
1	A	263[A]	VAL
1	A	263[B]	VAL
1	B	38	HIS
1	B	126	ASP
1	B	130	TRP
1	B	142	LEU

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Mol	Chain	Res	Type
1	B	221[A]	GLN
1	B	221[B]	GLN
1	C	38	HIS
1	C	126	ASP
1	C	130	TRP
1	C	142	LEU
1	C	221[A]	GLN
1	C	221[B]	GLN
1	D	38	HIS
1	D	126	ASP
1	D	130	TRP
1	D	142	LEU
1	D	221[A]	GLN
1	D	221[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	B	164	HIS
1	C	164	HIS
1	D	113	GLN
1	D	164	HIS
1	D	199	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HQD	A	1277	-	14,14,14	1.63	2 (14%)	18,20,20	1.78	5 (27%)
4	TAR	A	1278	-	9,9,9	0.87	0	12,12,12	1.11	0
3	HQD	B	1277	-	14,14,14	1.47	1 (7%)	18,20,20	1.67	4 (22%)
3	HQD	C	1277	-	14,14,14	1.50	1 (7%)	18,20,20	1.70	5 (27%)
4	TAR	C	1278	-	9,9,9	1.01	0	12,12,12	2.41	4 (33%)
4	TAR	C	1279[A]	-	9,9,9	1.50	3 (33%)	12,12,12	1.34	1 (8%)
4	TAR	C	1279[B]	-	9,9,9	1.27	1 (11%)	12,12,12	1.15	1 (8%)
4	TAR	C	1280	-	9,9,9	0.80	0	12,12,12	1.40	2 (16%)
3	HQD	D	1277	-	14,14,14	1.61	1 (7%)	18,20,20	1.46	3 (16%)
4	TAR	D	1278	-	9,9,9	0.97	0	12,12,12	1.93	4 (33%)
4	TAR	D	1279	-	9,9,9	1.22	0	12,12,12	1.58	5 (41%)
4	TAR	D	1280	-	9,9,9	1.14	0	12,12,12	1.83	3 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HQD	A	1277	-	-	0/0/0/0	0/0/2/2
4	TAR	A	1278	-	-	0/12/12/12	0/0/0/0
3	HQD	B	1277	-	-	0/0/0/0	0/0/2/2
3	HQD	C	1277	-	-	0/0/0/0	0/0/2/2
4	TAR	C	1278	-	-	0/12/12/12	0/0/0/0
4	TAR	C	1279[A]	-	-	0/12/12/12	0/0/0/0
4	TAR	C	1279[B]	-	-	0/12/12/12	0/0/0/0
4	TAR	C	1280	-	-	0/12/12/12	0/0/0/0
3	HQD	D	1277	-	-	0/0/0/0	0/0/2/2
4	TAR	D	1278	-	-	0/12/12/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TAR	D	1279	-	-	0/12/12/12	0/0/0/0
4	TAR	D	1280	-	-	0/12/12/12	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1277	HQD	C4-C10	5.09	1.48	1.40
3	B	1277	HQD	C4-C10	4.95	1.48	1.40
3	A	1277	HQD	C4-C10	4.23	1.47	1.40
3	C	1277	HQD	C4-C10	3.91	1.46	1.40
3	A	1277	HQD	C3-C2	-3.34	1.36	1.40
4	C	1279[B]	TAR	C2-C1	-2.80	1.49	1.52
4	C	1279[A]	TAR	O11-C1	-2.62	1.20	1.30
4	C	1279[A]	TAR	C2-C1	-2.35	1.49	1.52
4	C	1279[A]	TAR	C3-C4	-2.06	1.50	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1278	TAR	O41-C4-C3	4.65	127.44	113.89
3	B	1277	HQD	C3-C2-N1	4.54	121.87	117.55
3	A	1277	HQD	C3-C2-N1	4.35	121.69	117.55
4	C	1278	TAR	O3-C3-C2	3.95	118.38	110.19
4	D	1280	TAR	O41-C4-C3	3.91	125.30	113.89
3	C	1277	HQD	C8-C9-C10	-3.78	119.42	121.72
4	D	1278	TAR	O41-C4-C3	3.62	124.44	113.89
3	C	1277	HQD	C3-C2-N1	3.61	120.98	117.55
4	C	1278	TAR	O4-C4-C3	-3.60	110.61	121.15
3	D	1277	HQD	C3-C2-N1	3.55	120.93	117.55
3	A	1277	HQD	C8-C9-C10	-3.46	119.61	121.72
3	B	1277	HQD	O3-C3-C2	3.18	125.25	116.88
4	D	1278	TAR	O4-C4-C3	-3.06	112.19	121.15
3	D	1277	HQD	C8-C9-C10	-2.92	119.94	121.72
4	D	1280	TAR	O4-C4-C3	-2.80	112.96	121.15
4	C	1278	TAR	O11-C1-C2	2.73	121.84	113.89
4	D	1279	TAR	C3-C2-C1	2.71	117.02	109.90
4	D	1279	TAR	O41-C4-C3	2.70	121.76	113.89
3	A	1277	HQD	C5-C10-C9	2.69	119.46	117.79
3	A	1277	HQD	O3-C3-C2	2.67	123.90	116.88
3	B	1277	HQD	C8-C9-C10	-2.66	120.10	121.72
4	D	1278	TAR	C2-C3-C4	2.62	116.78	109.90
4	C	1280	TAR	O11-C1-C2	2.61	121.49	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1277	HQD	C5-C10-C9	2.53	119.36	117.79
4	D	1278	TAR	C3-C2-C1	2.42	116.26	109.90
3	D	1277	HQD	C5-C10-C9	2.35	119.24	117.79
4	C	1279[B]	TAR	O3-C3-C2	-2.29	105.44	110.19
4	C	1279[A]	TAR	O2-C2-C1	-2.21	105.98	110.73
3	A	1277	HQD	C-C2-C3	-2.19	121.00	123.13
4	C	1280	TAR	O2-C2-C3	-2.18	105.68	110.19
3	C	1277	HQD	C5-C10-C9	2.15	119.12	117.79
4	D	1279	TAR	O41-C4-O4	-2.10	119.31	124.07
3	C	1277	HQD	O3-C3-C2	2.09	122.38	116.88
4	D	1279	TAR	O2-C2-C3	-2.08	105.89	110.19
4	D	1280	TAR	C3-C2-C1	2.06	115.31	109.90
4	D	1279	TAR	O2-C2-C1	-2.06	106.32	110.73
3	C	1277	HQD	C4-C10-C9	2.04	121.28	118.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	273/287 (95%)	-0.01	1 (0%) 90 94	19, 32, 46, 76	0
1	B	273/287 (95%)	-0.12	2 (0%) 84 90	17, 26, 44, 63	0
1	C	273/287 (95%)	-0.09	2 (0%) 84 90	17, 28, 47, 64	0
1	D	272/287 (94%)	-0.10	2 (0%) 84 90	16, 28, 44, 61	0
All	All	1091/1148 (95%)	-0.08	7 (0%) 86 91	16, 28, 46, 76	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	275	GLY	3.9
1	D	4	THR	2.7
1	C	275	GLY	2.3
1	B	4	THR	2.2
1	C	24	ASP	2.1
1	D	26	ASP	2.0
1	B	13	ASP	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	TAR	D	1279	10/10	0.17	3.23	30,32,37,39	0
4	TAR	C	1279[B]	10/10	0.19	2.25	24,27,29,29	10
4	TAR	C	1279[A]	10/10	0.19	2.11	13,19,21,22	10
4	TAR	C	1280	10/10	0.13	1.09	24,30,33,36	0
3	HQD	B	1277	13/13	0.10	0.95	17,17,18,19	0
3	HQD	A	1277	13/13	0.11	0.88	21,22,24,24	0
4	TAR	A	1278	10/10	0.15	0.54	28,36,40,46	0
4	TAR	D	1280	10/10	0.11	0.41	22,28,31,32	0
3	HQD	C	1277	13/13	0.09	0.11	16,17,18,19	0
4	TAR	D	1278	10/10	0.12	0.05	25,30,34,40	0
3	HQD	D	1277	13/13	0.08	-0.41	18,19,21,21	0
4	TAR	C	1278	10/10	0.10	-0.50	23,31,36,39	0
2	K	A	1276	1/1	0.04	-2.31	33,33,33,33	0
2	K	C	1276	1/1	0.04	-2.42	31,31,31,31	0
2	K	B	1276	1/1	0.04	-2.60	25,25,25,25	0
2	K	D	1276	1/1	0.06	-3.73	28,28,28,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.